



## **A model to predict concentrations of DnBP metabolites in urine from a vapor-phase exposure**

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considering seasonal differences. As for some pollutants, e. g. benzene, assessment values are reached or exceeded, health effects cannot be excluded. Further monitoring and public health strategies targeted to parents of young children are warranted. Acknowledgements GerES IV was funded by the German Ministry of Education and Research and the Ministry for the Environment, Nature Conservation, Building and Nuclear Safety. GerES IV field work was carried out by the Robert Koch Institute.

Keywords: A-exposure models, A-exposure factors, B-VOCs, C-indoor, D-children

### We-O-C3-02

#### **A model to predict concentrations of DnBP metabolites in urine from a vapor-phase exposure**

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**Abstract:** Six volunteers spent 6 hours in an exposure chamber on 2 separate occasions during which the air contained elevated levels of DnBP. For both sessions, volunteers were only clad in shorts, facilitating the air-to-skin transfer of DnBP. In one of the sessions, the volunteers breathed clean air from an airtight helmet, restricting exposure to the dermal pathway. In the other session, they did not wear the helmet and exposure was via both inhalation and dermal pathways. One urination event occurred during the chamber exposure, and all volunteers collected full urine samples for 50 hours after leaving the chamber. Levels of DnBP metabolites in the urine were above background while in the chamber and for about 36 hours after leaving the chamber. These experiments indicated that the contribution of the dermal pathway to DnBP uptake was roughly 80% of the inhalation pathway. Prior to these experiments, a transient air-to-skin-to-blood model had been published. A separate publication described a simple pharmacokinetic (PK) model to predict urine concentrations of DnBP metabolites following an oral exposure. The transient air-to-skin-to blood model was applied to this experiment to predict the flux of DnBP to blood and linked with the PK model predicting the appearance of DnBP metabolites in urine. When applied to the data set, it was found that the model reasonably predicted the urine concentrations for the urine event in the chamber and the first few events upon leaving the chamber, but then the linked model began over-predicting metabolite excretions by roughly an order of magnitude. It is believed that when participants donned clothing after leaving the chamber, some of the residual DnBP sorbed in the skin was removed by the clothing; this sink was not accounted for in the linked model. This presentation will review the experiments, the data and models, and the linked model results. Efforts to develop a clothing removal algorithm will be summarized.

Keywords: B-phthalates, A-biomonitoring, C-air, A-exposure models

### We-O-C3-03

#### **Development and Evaluation of an ADME-informed High Throughput Exposure Estimation Tool**

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**Abstract:** EPA's Chemical Safety for Sustainability (CSS) research program has been developing new ways to prioritize chemicals used in consumer products and articles. Using a risk-based methodology to account for both toxicity and exposure offers a comprehensive and systematic approach toward prioritization. The purpose of this prioritization initially is to identify those chemicals for which typical product usage rates may lead to undesirable exposures, and ultimately to identify potentially problematic chemicals before they even reach the marketplace. We developed a flexible dashboard-type chemical prioritization tool that ranks exposures from consumer products accounting for product formulation and use; physical-chemical properties (e.g., partitioning coefficients); and user exposure factors, activity patterns, and product use profiles. Additionally, the tool incorporates route- and chemical-specific internal dose predictions that consider absorption, distribution, metabolism, and excretion (ADME) processes allowing for better comparison of toxicity and exposure estimates. The tool indicates products likely to be in specific microenvironments, along with the ways people will contact chemicals in these products, thus allowing better screening and ranking of exposure in a high throughput environment. Currently, the tool considers seven pathways of exposure for 451 chemicals present in 946 separate consumer products with the ability to add more chemicals and products as information becomes available. In this presentation, the tool is evaluated by comparing the predicted rank order of chemical